MODELING, SIMULATION AND OPTIMIZATION IN ENERGY SYSTEMS

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Summary

Concern about the depletion of physical and economic resources as well as the degradation of the environment due to the construction and operation of energy systems makes it necessary to design and operate such systems in such a way that they not only cover the energy needs of the consumers, but also do this with the minimum

consumption of resources and have adverse effects on the environment. Thus, optimization methods have to be developed and applied. A prerequisite for this purpose is a deep understanding of the phenomena and processes, the development of their proper phenomenological and mathematical models, and the simulation that will derive the values of variables characterizing the performance of the system. Modeling, simulation and optimization methods as well as application examples are presented in the various articles of the present Topic, while the text here serves as a brief introduction, accompanied by a description of the present state of the art and of future research needs in the field.

1. Introduction

Energy systems (i.e. systems that convert one or more energy fluxes into other energy fluxes of different type), no matter whether primitive or elaborate, have been built and operated since antiquity. Power plants, cogeneration systems (e.g., combined heat and power systems), propulsion plants, chemical plants, heating systems, cooling systems, refrigeration systems and air conditioning systems are examples of energy systems. The concept can be broadened to include on the one hand units or systems of energy transfer (e.g. heat exchangers, networks for transportation of electricity and heat) and on the other hand systems for covering energy needs at the level of a region or a country (e.g., a system with several power plants and a network that supplies a country with electricity).

The main concern of a designer and a manufacturer is to design and build a system with a pre-specified capacity that can cover the energy needs of the consumer(s). In the past, simply achieving the pre-specified capacity was sufficient, while efficiency or cost were of secondary importance. Today the task is much more demanding: the main goal (e.g. capacity) must be achieved, but with the maximum possible positive effects (e.g., efficiency, revenue, social benefits) and/or the minimum possible adverse effects (e.g., fuel consumption, costs, environmental degradation). The complexity of most modern systems and processes is such that the search for the maximum or the minimum of a performance criterion may not be performed effectively unless mathematical procedures known by the general name “optimization” are used. In order for these procedures to be applied, there is a need to first construct a mathematical model, which describes the performance of the energy system as closely as possible, and then, based on this model, to develop a simulation procedure (usually implemented in a computer algorithm) that will produce numerical values of the performance parameters of the system. These parameters may reveal the thermodynamic performance (efficiency, fuel consumption, etc.), the economic performance (e.g. cost of energy products) or the environmental performance (e.g. emission of pollutants) of the system. These subjects are treated in the present Topic. An overview is presented in the following, while detailed information is given in the individual articles.

2. Modeling and Simulation of Energy Systems

2.1. Definition of Modeling and Simulation

Modeling and simulation are two distinct aspects of the design problem:

- ***Modeling** is the act of interpreting a set of physical phenomena and of devising a reasonably complete, closed and comprehensive phenomenological and mathematical formulation for its description*. Such a description usually results in a system of equations that, given a suitable set of initial data, can be solved to yield the values of the variables that describe the physics of the phenomena subject to modeling. Modeling is a dynamic concept: the improvement of our comprehension of the physics underlying a certain set of phenomena leads to successive refinements of previous models resulting in a more general, or more precise, agreement with the perceived reality of a process. A model can thus be seen as a *paradigm of reality,* in the sense that it expresses our interpretation of a myriad of interrelated micro- and macro effects that constitute the "real" process.
- ***Simulation** is the act of putting the models to work*. On the basis of some suitable initial data about the state of the system and its environment, a proper mathematical formulation deriving from the model is applied to obtain the numerical values of all relevant variables for the problem in case.

2.2. A Brief History of Energy Systems Design Procedures

Energy conversion systems have been in use since the late Bronze Age, and there are well-documented examples of relatively advanced devices constructed 4000 years ago. In Mesopotamia (the region presently spanned by modern Iran and Iraq), wind-to-mechanical energy conversion performed by means of primitive, but very ingenious, windmills provided the motive power needed for milling wheat. Similar windmills were known throughout the eastern Mediterranean area, and possibly even in India and China. For the same purpose, Babylonians and perhaps also ancient Indian civilizations performed hydraulic-to-mechanical energy conversion via rudimentary water wheels. Even thermal-to-mechanical energy conversion was enacted: the drawings by Hero (second century BC) show that an impulse steam turbine was in use in Egypt at least as far back as the fifth century BC. The design of such devices was certainly non-systematic, trial and error being the common design technique. The "engineers" of that time were regarded rather as magicians; they constituted a closed social class and passed their experience from generation to generation without leaving any written physical explanation of the phenomena they were exploiting (except possibly for some symbolically encrypted knowledge). In modern terms, we can say that they did not leave records of the models they used: of course, there was not even the notion of simulation. Roman engineers, for instance, left no written record of their design practices for any of the many hydraulic plants they built. It was only after the Middle Ages (roughly, after 1300) that the first "scientific" explanations were attempted: we could say that "modeling" was born then.

From the fifteenth to the seventeenth century, windmills, watermills, and some rudimentary thermal systems (gunpowder was brought to the West from China after the year 1400) were developed, always on a trial and error basis, but often with extraordinary insight on the part of individual inventors. Design was still based on an elementary modeling activity, and no simulation was even conceived. Things changed substantially after the development of the first steam engines in the second half of the eighteenth century: the science of thermodynamics was born, and the extraordinary pace of development of the original concept in literally hundreds of applications reveals a titanic effort on the part of engineers to understand the underlying physical principles, and to concoct a "model" of their systems. Heat transfer began to be understood, and a strenuous modeling activity saw the light. Concepts such as latent and specific heat, energy transfer by conduction and convection, and fluid motion were intensely studied in the eighteenth century: of course, this had to be based on an extended "phenomenological modeling". If we examine the construction details of the machines of that age, we see that the physics of several phenomena (leakages, fluid motion, mechanical friction, and so on) were quite well understood, in that proper models were used in the design and operation of the systems.

From the mid-eighteenth to the early twentieth century, the fundamental works of Lavoisier, Carnot, Gouy, Stodola, and many others led to an evermore exact understanding of the physical laws governing the phenomena of heat and work transfer, and modeling became a scientific activity, based not only on intuition but on exact and physically sound rules involving mass and energy balances, and even consideration of irreversible losses.

In the twentieth century, emphasis was put on the organization of the large body of experimental evidence previously acquired, and models became systematic: that is, based on universal conservation equations and on the proper application of general thermo-physical property relations. Processes and systems (notably, chemical and thermal) were designed on the basis of ever more refined models of the underlying phenomena, and design procedures were devised that made use of the mathematical formulation of these models to derive (by hand calculation!) some of the independent variables. Simulation was born and immediately adapted to those rather inefficient tools: iterative calculations were reduced to a minimum, and widespread use was made of abaci and tables for relating one design variable to another. Only after the computer made its appearance in the engineering world (the event can be dated to1936, when the first "electronic" computer, the Z1, was switched on by Konrad Zuse in Saarbrucken) was it possible to transfer the tedious load of iterative calculations from humans to machines. It became immediately apparent that computer-assisted procedures were more precise, less prone to casual error, and much faster than human calculations. The age of the slide rule came to an end, and the computer became a necessary design tool for process and design engineers.

In recent decades, the performance of every computing device has grown at an impressive pace: number of operations per unit time (FLOPS), storage size (working "memory"), input–output devices, reliability and portability, and user friendliness have reached levels today that were almost unthinkable in the late 1980s, and progress is made literally every day. This led of course to the development of specific engineering applications. Computer tools are now available for process simulation, for the design (sizing) of components and structures, for process monitoring and control, and so on. The trend has accelerated to the point that it is difficult today to perform a flow-sheet activity (or any kind of design calculation!) without some sort of computer aid. Recent developments include the complete automation of simulation procedures and the shifting of some of the modeling activity from the human mind to the artificial assistant (see *Artificial Intelligence in Process Design*). Computer procedures are presently used for the solution of design and optimization engineering problems, and the trend is clearly towards the codification of the “creative” portion of the design activity into some sort of “intelligent” code.

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Biographical Sketches

Christos A. Frangopoulos (born July 28, 1948) is Professor at the Department of Naval Architecture and Marine Engineering, National Technical University of Athens (NTUA), Greece. He received the Diploma in Mechanical and Electrical Engineering from the NTUA in 1971. After his military service (1971-1973), he worked as Superintendent Engineer of ship-owning companies, and as Head of the Diagnostic Center of a ship repairing company in Greece (1973-1979). He performed graduate studies in Mechanical Engineering with major in Thermal Sciences at the Georgia Institute of Technology, Atlanta, Ga., USA, leading to the M.Sc. degree (1980) and Ph.D. degree (1983). He joined the Department of Naval Architecture and Marine Engineering (NTUA) as a faculty member in 1985. He lectures on marine engineering, as well as marine and land-based energy systems in both undergraduate and inter-departmental graduate courses. His research activity is related to the development and application of methods for analysis, evaluation and optimal synthesis, design and operation of energy systems (power plants, propulsion plants, heat recovery systems, cogeneration systems, etc.) by combining thermodynamic, economic and environmental considerations. Second Law (exergetic) analysis and internalization of environmental externalities are two particular subjects of this work. He has often given invited lectures on the results of his research in several countries. Among his publications are more than fifty papers in journals and international conferences, one book on cogeneration (in Greek) and an educational material on cogeneration (in English) available in electronic form on the web.

Enrico Sciubba (born July 11, 1949) is a Professor in the Department of Mechanical and Aeronautical Engineering of the University of Roma 1 “La Sapienza”, in Roma, Italy. He received a M.Eng. Degree in Mechanical Engineering from U. of Roma in 1972. After working for two years (1973-75) as a Research Engineer in the Research & Development Division of BMW, Munich (Germany), he returned to the University of Roma as a Senior Researcher (1975-1978). He then enrolled in the Graduate School of Mechanical Engineering, majoring in Thermal and Fluid Sciences, at Rutgers University, Piscataway, NJ, USA, where he was granted a Ph.D. degree in 1981. He joined the Department of Mechanical Engineering of the Catholic University of America, in Washington DC, USA, as an Assistant Professor in 1981, and worked there until 1986, when he returned to the University of Roma 1 first as a Lecturer, then as an Associate and finally Full Professor. He holds the Chair of Turbomachinery, and lectures on Energy Systems as well, both at the undergraduate and graduate level. In 1999 Dr. Sciubba was elected a Fellow of the American Society of Mechanical Engineers. In 2000, he also received a Honorary Doctoral title from the University Dunarea de Jos of Galati (Romania). His research is related to CFD of Turbomachinery, to Exergy Analysis, and to Artificial Intelligence applications in the design of Energy Systems. His publications include more than 30 archival papers, over 100 articles in international conferences, one book on Turbomachinery (in Italian) and one on Artificial Intelligence (in English).